Hyper-Parallel Tempering Monte Carlo Method and Its Applications

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A new generalized hyper-parallel tempering Monte Carlo molecular simulation method is presented for study of complex fluids. The method is particularly useful for simulation of many-molecule complex systems, where rough energy landscapes and inherently long characteristic relaxation times can pose formidable obstacles to effective sampling of relevant regions of configuration space. The method combines several key elements from expanded ensemble formalisms, parallel-tempering, open ensemble simulations, configurational bias techniques, and histogram reweighting analysis of results. It is found to accelerate significantly the diffusion of a complex system through phase-space.

In this presentation, we demonstrate the effectiveness of the new method by implementing it in grand canonical ensembles for a Lennard-Jones fluid, for the restricted primitive model of electrolyte solutions (RPM), and for polymer solutions and blends. Our results indicate that the new algorithm is capable of overcoming the large free energy barriers associated with phase transitions, thereby greatly facilitating the simulation of coexistence properties. It is also shown that the method can be orders of magnitude more efficient than previously available techniques. More importantly, the method is relatively simple and can be incorporated into existing simulation codes with minor efforts.